Achieving renormalization—scale— and scheme—independence in Padé—related resummation in QCD

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Abstract

Previously developed Padé–related method of resummation for QCD observables, which achieves exact renormalization–scale–invariance, is extended so that the scheme–invariance is obtained as well. The dependence on the leading scheme parameter c_2 is eliminated by a variant of the method of the principle of minimal sensitivity. The subleading parameter c_3 in the approximant is then fixed in such a way that the correct known location of the leading infrared renormalon pole is reproduced. Thus, β –functions which go beyond the last perturbatively calculated order in the observable are used. The β –functions in the approximant are quasianalytically continued by Padé approximants. Two aspects of nonperturbative physics are accounted for in the presented resummation: a mechanism of quasianalytic continuation from the weak– into the strong–coupling regime, and the (approximant–specific) contribution of the leading infrared renormalon. The case of the Bjorken polarized sum rule is considered as a specific example of how the method works. PACS number(s): 11.10.Hi, 11.80.Fv, 12.38.Bx, 12.38.Cy

I. INTRODUCTION

In QCD, as a result of extensive perturbative calculations, some observables are now known to the next-to-next-to-leading order (NNLO, $\sim a^3$) in the power expansion in the strong coupling parameter $a \equiv \alpha_s/\pi$. Knowing such truncated perturbation series (TPS), the question of their resummation is gaining importance, especially if the typical process energies associated with the observable are low and thus the relevant coupling parameter is large. In such cases, it is to be expected that additional perturbative and nonperturbative effects, not explicitly contained in the TPS, will be numerically important. Many methods of resummation, based on the available TPS, try to incorporate such effects. Some of these methods eliminate the dependence on the renormalization scale (RScl) and scheme (RSch) by fixing them in the TPS itself in a judicious way – these methods could be regarded as renormalization–group–improved methods of resummation: BLM–fixing motivated by the

large- n_f considerations [1], Stevenson's principle of minimal sensitivity (PMS) [2], Grunberg's effective charge method (ECH) [3] (cf. Ref. [4] for a related method). Some of the recent works on resummations are the method of "commensurate scale relations" and related approaches [5], a method using an analytic form of the coupling parameter [6], ECH-related approaches [7], and an expansion in the two-loop coupling parameter [8]. In the past few years, Padé approximants (PA's) were also shown to be a rather successful method of resummation [9], especially since the resummed results show in general weakened RScl- and RSch-dependence. The diagonal Padé approximants (dPA's) are particularly well motivated for observables since they are RScl-independent in the approximation of the one-loop evolution of the coupling $\alpha_s(Q^2)$ [10]. In addition, PA's go in their form beyond the polynomial form of the TPS on which they are based, thus contain a strong mechanism of quasianalytic continuation from the weak- into the strong-coupling regime, and can consequently incorporate some of the nonperturbative effects into the resummed result.

Recently, an extension of the method of dPA's was presented [11] which leads to the exact perturbative RScl-independence of the resummed result. We then extended the method so that it is applicable also to NNLO TPS's [12], and suggested there a way to fix the RSch by applying the principle of minimal sensitivity (PMS). The way suggested in [12] does not work properly in practice since no minimum of the PMS equation $\partial A/\partial c_2 = 0$ [Eq. (40) there] exists. The dependence of our approximants on the RSch-parameters c_2 and c_3 of the original TPS is a significant problem when the approximants are applied to the low-energy observables like the Bjorken polarized sum rule (BjPSR) at low $Q_{\rm photon} \approx \sqrt{3}$ GeV [13].

This problem is addressed in the present paper. For the case of NNLO TPS, an extended version \mathcal{A} of our approximant is constructed where the dependence on the leading RSch-parameter c_2 is eliminated by a variant of the PMS. Subsequently, the sub-leading RSch-parameter c_3 is adjusted so that the approximant reproduces the correct location of the leading infrared renormalon pole. The latter procedure is carried out in the concrete example of the BjPSR. The same method of c_3 -fixing is then applied to Grunberg's ECH and Stevenson's TPS-PMS approximants. Hence, in the approximants we use β -functions which go beyond the last perturbatively calculated order in the observable (NNLO). Further, a PA-type of quasianalytic continuation for the β -functions is used in all these approximants. The resulting predictions for $\alpha_s^{\overline{\text{MS}}}(M_Z^2)$ from the BjPSR are presented, along with those when PA's are applied to the BjPSR, and compared with the world average. Differences between between our approximant and the other methods (ECH, TPS-PMS; PA's) are pointed out.

II. CONSTRUCTION OF C_2 -INDEPENDENT APPROXIMANTS

Consider a QCD observable S with negligible mass effects and known NNLO TPS

$$S_{[2]} = a_0(1 + r_1 a_0 + r_2 a_0^2) , (1)$$

with:
$$a_0 \equiv a(\ln Q_0^2; c_2^{(0)}, c_3^{(0)}, \cdots)$$
, $r_1 = r_1(\ln Q_0^2)$, $r_2 = r_2(\ln Q_0^2; c_2^{(0)})$. (2)

We denoted $a \equiv \alpha_s/\pi$; Q_0 is the Euclidean RScl; $c_j^{(0)}$ $(j \ge 2)$ are the RSch-parameters used in the TPS. The coupling parameter $a(\ln Q^2; c_2^{(0)}, \ldots)$ in this RSch evolves according to the renormalization group equation (RGE) $\partial a/\partial \ln Q^2 = \beta(a; c_2^{(0)}, c_3^{(0)}, \ldots)$. Here, the β -function

has the power expansion $\beta(a) = -\beta_0 a^2 (1 + c_1 a + c_2^{(0)} a^2 + c_3^{(0)} a^3 + \cdots)$, and β_0 and c_1 are RScl-and RSch-invariant. This RGE can be integrated (see Appendix of [2])

$$\beta_0 \ln \left(\frac{Q_0^2}{\tilde{\Lambda}^2} \right) = \frac{1}{a_0} + c_1 \ln \left(\frac{c_1 a_0}{1 + c_1 a_0} \right) + \int_0^{a_0} dx \left[\frac{1}{x^2 (1 + c_1 x)} + \frac{\beta_0}{\beta(x; c_2^{(0)}, c_3^{(0)} \dots)} \right] , \qquad (3)$$

where $a_0 \equiv a(\ln Q_0^2; c_2^{(0)}, c_3^{(0)}, \ldots)$ and $\tilde{\Lambda}$ is a universal scale (~ 0.1 GeV). When subtracting (3) from the analogous equation for $a \equiv a(\ln Q^2; c_2, c_3, \ldots)$, an equation is obtained which relates a with a_0 , i.e., determines a in terms of a_0 . This equation then determines also the expansion of a in powers of a_0 . From now on, we fix the " Λ -convention" to $\Lambda = \tilde{\Lambda}$.

We make the following ansatz for our approximant, motivated by the RScl-invariant (but not RSch-invariant) approximant of Refs. [12,13]:

$$\sqrt{\mathcal{A}_{S^2}} = \left\{ \tilde{\alpha} \left[a(\ln Q_1^2; c_2^{(1)}, c_3^{(1)}, \ldots) - a(\ln Q_2^2; c_2^{(2)}, c_3^{(2)}, \ldots) \right] \right\}^{1/2} \left(= S_{[2]} + \mathcal{O}(a_0^4) \right) , \qquad (4)$$

where we regard now the parameters $c_2^{(j)}, c_3^{(j)}, \dots$ (j=1,2) as fixed numbers, and $c_2^{(1)} \neq c_2^{(2)}$. Five parameters in the approximant $(\tilde{\alpha}, Q_1^2, Q_2^2, c_2^{(1)}, c_2^{(2)})$ can be fixed by applying five conditions to the approximant. Three conditions are obtained from the so called minimal requirement: When we expand the approximant back in powers of a_0 , the first three coefficients of the original TPS (1) have to be reproduced. The additional two conditions are obtained by a variant of the PMS

$$(\partial \mathcal{A}_{S^2}/\partial c_2^{(1)})|_{c_2^{(2)}} \sim a_0^6 \sim (\partial \mathcal{A}_{S^2}/\partial c_2^{(2)})|_{c_2^{(1)}}$$
 (5)

This allows us to fix $c_2^{(j)}$'s. If we took in (4) $c_2^{(1)} = c_2^{(2)}$ ($\equiv c_2$), and $c_k^{(1)} = c_k^{(2)}$ ($k \geq 3$), i.e., the approximants of [12,13], we would obtain $\partial \mathcal{A}_{S^2}/\partial c_2 = -10c_1a_0^5 + \mathcal{O}(a_0^6) \not\sim a_0^6$, i.e., the PMS condition would not be satisfied. This is the main reason why we take two different (leading) parameters $c_2^{(j)}$ in the two a's in (4). Further, since the two energy scales in (4), and in the approximants of [12,13], are $Q_1^2 \neq Q_2^2$, it does not appear unnatural to have $c_2^{(1)} \neq c_2^{(2)}$. But the (subleading) parameters $c_3^{(j)}$ cannot be fixed by such an approach since

$$(\partial \mathcal{A}_{S^2}/\partial c_3^{(s)})|_{\delta c_3} = 2a_0^5 + \mathcal{O}(a_0^6)$$
 where $: c_3^{(s)} \equiv (c_3^{(1)} + c_3^{(2)})/2, \ \delta c_3 \equiv (c_3^{(1)} - c_3^{(2)})$. (6)

The same problem arises in the NNLO polynomial approximants ECH and TPS-PMS where $\partial \mathcal{A}_{\mathcal{S}}/\partial c_3 = (1/2)a_0^4 + \mathcal{O}(a_0^5) \ [\Rightarrow \partial (\mathcal{A}_{\mathcal{S}})^2/\partial c_3 = a_0^5 + \mathcal{O}(a_0^6)].$ We will take, for simplicity, $c_3^{(1)} = c_3^{(2)} \equiv c_3$, and the value of c_3 will be fixed later.

Conditions (5) then depend also on $\delta c_4 \equiv (c_4^{(1)} - c_4^{(2)})$ which we set equal to zero to avoid further (presumably unnecessary) complications. Then the set of the five equations determining $\tilde{\alpha}$, Q_j^2 and $c_2^{(j)}$ (j=1,2) reads

$$y_{-}^{4} - y_{-}^{2} z_{0}^{2}(c_{2}^{(s)}) + y_{-} \frac{5}{4} c_{1} \delta c_{2} - \frac{3}{16} (\delta c_{2})^{2} = 0 ,$$
 (7)

$$\left\{27(\delta c_2)^3 - 157c_1(\delta c_2)^2 y_- - 8\delta c_2 y_-^2 \left[-27c_1^2 + 12c_2^{(s)} + 34y_-^2 - 8z_0^2(c_2^{(s)}) \right] \right\}$$

$$+48c_1y_-^3 \left[13y_-^2 - 3z_0^2(c_2^{(s)})\right] \left\{ \left[5c_1\delta c_2 + 16y_-^3 - 8z_0^2(c_2^{(s)})y_-\right)\right]^{-1} = 0, \tag{8}$$

$$\left\{ 27(\delta c_{2})^{4} - 315c_{1}(\delta c_{2})^{3}y_{-} + 64z_{0}^{4}(c_{2}^{(s)})y_{-}^{2} \left[7c_{1}^{2} - 2c_{2}^{(s)} + 3z_{0}^{2}(c_{2}^{(s)}) \right] - 4\delta c_{2}(20c_{1}y_{-} - 3\delta c_{2}) \right. \\
\left. \times \left[-2c_{2}^{(s)}y_{-}^{2} - 2c_{2}^{(s)}z_{0}^{2}(c_{2}^{(s)}) + 12z_{0}^{2}(c_{2}^{(s)})y_{-}^{2} + 3z_{0}^{4}(c_{2}^{(s)}) + 7c_{1}^{2}\left(y_{-}^{2} + z_{0}^{2}(c_{2}^{(s)})\right) \right] \right. \\
\left. + 36(\delta c_{2})^{2}y_{-}^{2} \left[z_{0}^{2}(c_{2}^{(s)}) + 25c_{1}^{2} \right] \right\} \left[5c_{1}\delta c_{2} + 16y_{-}^{3} - 8z_{0}^{2}(c_{2}^{(s)})y_{-} \right]^{-1} = 0 , \tag{9}$$

$$-r_1 + \frac{1}{2}c_1 - \frac{1}{4}\frac{\delta c_2}{y_-} = y_+ , \qquad \tilde{\alpha} = -\frac{1}{2y_-} , \qquad (10)$$

where we use notations

$$y_{\pm} \equiv \frac{1}{2}\beta_0 \left[\ln \frac{Q_1^2}{Q_0^2} \pm \ln \frac{Q_2^2}{Q_0^2} \right] , \quad \delta c_2 \equiv c_2^{(1)} - c_2^{(2)} , \quad c_2^{(s)} \equiv \frac{1}{2} (c_2^{(1)} + c_2^{(2)}) , \quad (11)$$

$$z_0^2 \equiv \left(2\rho_2 + \frac{7}{4}c_1^2\right) - 3c_2^{(s)} \equiv z_0^2(c_2^{(s)}) , \qquad \rho_2 = r_2 - r_1^2 - c_1r_1 + c_2^{(0)} . \tag{12}$$

Here, ρ_2 is an RScl- and RSch-invariant, and therefore it is straightforward to see that the solutions of the system (7)–(10) for Q_j^2 and $c_2^{(j)}$ (j=1,2) and for $\tilde{\alpha}$ are independent of the original choice of the RScl (Q_0^2) and of the RSch $(c_2^{(0)}, c_3^{(0)}, \ldots)$. Eqs. (8)–(9) originate from PMS conditions (5), and the other three identities from the minimal condition. In particular, the latter three identities (7) and (10) show that $\tilde{\alpha}$ and the scales Q_1^2 and Q_2^2 are Q_0^2 -independent irrespective of whether $\delta c_2 \neq 0$ or $\delta c_2 = 0$.

The coupled system of three equations (7)–(9) for the three unknowns $c_2^{(j)}$ (j=1,2) and $y_- \equiv \beta_0 \ln(Q_1/Q_2)$ can be solved numerically. The solutions which give $|\tilde{\alpha}| \ll 1$ or $|\tilde{\alpha}| \gg 1$ must be discarded because they would cause numerical instabilities in the approximant, and they would not make sense physically either – one of the scales Q_1 , Q_2 would be orders of magnitude different from the other. There are apparently two possibilities: 1.) y_- , $c_2^{(s)}$ and δc_2 are all real numbers; 2.) $c_2^{(s)}$ is real, y_- and δc_2 are imaginary numbers. In both cases, the approximant itself would be real, as it shoud be.

If there are several solutions which give different values for the approximant, we should choose (again within the PMS-logic) among them the solution with the smallest curvature with respect to $c_2^{(1)}$ and $c_2^{(2)}$.

III. APPLICATION TO THE BJORKEN POLARIZED SUM RULE; C_3 -FIXING

The Bjorken polarized sum rule (BjPSR) involves the isotriplet combination of the first moments over $x_{\rm Bj}$ of proton and neutron polarized structure functions

$$\int_0^1 dx_{\rm Bj} \left[g_1^{(p)}(x_{\rm Bj}; Q_{\rm ph}^2) - g_1^{(n)}(x_{\rm Bj}; Q_{\rm ph}^2) \right] = \frac{1}{6} |g_A| \left[1 - S(Q_{\rm ph}^2) \right] , \qquad (13)$$

where $p^2 = -Q_{\rm ph}^2 < 0$ is γ^* momentum transfer. At $Q_{\rm ph}^2 = 3 {\rm GeV}^2$ where three quarks are assumed active $(n_f = 3)$, and if taking $\overline{\rm MS}$ RSch and RScl $Q_0^2 = Q_{\rm ph}^2$, we have [14,15]:

$$S_{[2]}(Q_{\rm ph}^2; Q_0^2 = Q_{\rm ph}^2; c_2^{\overline{\rm MS}}, c_3^{\overline{\rm MS}}) = a_0(1 + 3.583a_0 + 20.215a_0^2) ,$$
 (14)

with:
$$a_0 = a(\ln Q_0^2; c_2^{\overline{\text{MS}}}, c_3^{\overline{\text{MS}}}, \dots)$$
, $n_f = 3$, $c_2^{\overline{\text{MS}}} = 4.471$, $c_3^{\overline{\text{MS}}} = 20.99$. (15)

Solving numerically the system of equations (7)–(10), we obtain one solution only

$$c_2^{(1)} = 1.465$$
, $c_2^{(2)} = 5.137$, $Q_1 = 0.594 \text{ GeV}$, $Q_2 = 1.164 \text{ GeV}$ ($\Rightarrow \tilde{\alpha} = 0.3301$). (16)

This solution is independent of the choice of RScl and RSch. For the time being, we will set the higher parameters $c_k^{(j)} = 0$ ($k \ge 4$, j = 1, 2). Now our approximant depends only on the still free parameter c_3 . This dependence is numerically significant. For a typical value $a_0 = 0.09$ [$\Rightarrow \alpha_s^{\overline{\text{MS}}}(3\text{GeV}^2) \approx 0.283$, $\alpha_s^{\overline{\text{MS}}}(M_Z^2) \approx 0.113$], the approximant (4) gives 0.1523 and 0.1632 when $c_3 = 0$, $c_3^{\overline{\text{MS}}}$, respectively, i.e. a difference of 7.2%. In the case of the ECH and TPS-PMS approximants for the BjPSR, the respective differences are 3.8% and 4.0%.

Parameter c_3 characterizes the N³LO term in the corresponding β -functions [cf. Eq. (3)], and information on its value cannot be obtained from the NNLO TPS [cf. Eq. (6)]. Therefore, to fix c_3 , we should incorporate into the approximants a known piece of (nonperturbative) information beyond the NNLO TPS (14). Natural candidates for this are the known locations of the poles [16,17] of the leading infrared renormalon (IR₁: $z_{\text{pole}} = 1/\beta_0$) or ultraviolet renormalon (UV₁: $z_{\text{pole}} = -1/\beta_0$), i.e., the poles of the Borel transform $B_S(z)$ of S closest to the origin. Large- β_0 evaluations [17], based on the formulas of [16] and using simple Borel transforms in a variant of the V-scheme (RScl $Q_0 = Q_{\text{ph}} \exp(-5/6)$) and one-loop-evolved a), suggest that the UV₁ contributions to the BjPSR at $Q_{\text{ph}}^2 = 2$ -3 GeV² are suppressed in comparison to the IR₁ contributions by a factor 3-4 (cf. their Fig. 2).

Therefore, we will fix c_3 in the three approximants by incorporating in them the information on the location of the IR₁ pole $z_{\text{pole}} = 1/\beta_0$ (=4/9). For that, we employ RScl– and RSch–invariant Borel transforms. Simple Borel transforms are not RScl/RSch–invariant, the use of their TPS's leads to RScl/RSch–dependent c_3 –fixing, which we want to avoid. We use a variant of the invariant Borel transform B(z) introduced by Grunberg [18], who in turn introduced it on the basis of the modified Borel transform of Ref. [19]

$$S(Q_{\rm ph}^2) = \int_0^\infty dz \exp\left[-\rho_1(Q_{\rm ph}^2)z\right] B_S(z) ,$$
 (17)

where ρ_1 is the first RScl/RSch-invariant [2] of S: $\rho_1 = -r_1 + \beta_0 \ln(Q_0^2/\tilde{\Lambda}^2) = \beta_0 \ln(Q_{\rm ph}^2/\tilde{\Lambda}^2)$. Here, $\tilde{\Lambda}$ is the universal scale of Eq. (3), and $\bar{\Lambda}$ a scale which depends on the choice of S but is RScl/RSch-invariant and $Q_{\rm ph}$ -independent. The $\rho_1(Q_{\rm ph}^2)$ is, up to an additive constant (the latter not affecting the poles of B_S), equal to $1/a^{(1-\text{loop})}(Q_{\rm ph}^2)$. Thus, $B_S(z)$ of (17) reduces to the simple Borel transform, up to a factor $\exp(cz)$, once higher than one-loop effects are ignored. The coefficients of the power expansion of $B_S(z)$ of (17) are RScl/RSch-invariant, in contrast to the case of the simple Borel transform. These invariant coefficients can be related with coefficients r_n of S most easily in a specific RSch $c_k = c_1^k$ ($k \ge 2$)

$$B_S(z) = (c_1 z)^{c_1 z} \exp(-r_1 z) \sum_{0}^{\infty} \frac{(\tilde{r}_n - c_1 \tilde{r}_{n-1})}{\Gamma(n+1+c_1 z)} z^n \equiv (c_1 z)^{c_1 z} \overline{B}_S(z) . \tag{18}$$

Here, \tilde{r}_n is the coefficient at \tilde{a}^{n+1} in the expansion of S in powers of $\tilde{a} \equiv a(\ln Q_0^2; c_1^2, c_1^3, ...)$; by definition $\tilde{r}_{-1} = 0$, $\tilde{r}_0 = 1$. Thus, the expansion of the approximant $\sqrt{A_{S^2}}(c_3)$ in powers of \tilde{a} leads to the expansion of the (reduced) Borel transform $\overline{B}_{\sqrt{\mathcal{A}}}(z)$ in powers of z. The coefficients starting at z^3 are predictions of the approximant and c_3 -dependent: $\overline{B}_{\sqrt{\mathcal{A}}}(z) = 1 + \bar{b}_1 z + \bar{b}_2 z^2 + \bar{b}_3 z^3 + \cdots$, with $\bar{b}_1 \approx -0.7516$, $\bar{b}_2 \approx 0.4209$, $\bar{b}_3 \approx (-2.664 + 0.1667c_3)$, etc. Terms

with high powers of z are not reliable, because the approximant is based on an NNLO TPS $S_{[2]}$ with only two terms beyond the leading order. We then employ Padé approximants (PA's) of power expansion of $\overline{B}_{\sqrt{\mathcal{A}}}$, since they are efficient in determining the pole structure of $\overline{B}_{\sqrt{\mathcal{A}}}$. We performed the expansion of $\sqrt{\mathcal{A}}(c_3)$ up to $\sim \tilde{a}^7$, obtaining the expansion of $\overline{B}_{\sqrt{\mathcal{A}}}(z)$ up to $\sim z^6$. This allowed us to construct $\operatorname{PA}_{\overline{B}}$'s of as high order as [3/3] or [4/2]. The value of c_3 in $\operatorname{PA}_{\overline{B}}$ was then adjusted to achieve $z_{\operatorname{pole}} = 1/\beta_0$ (= 4/9). The resulting values of c_3 are presented in the second column (TPS_{\beta}) of Table I. We carried out the

$PA_{\overline{B}}$	$c_3 (\sqrt{\mathcal{A}_{S^2}})$: TPS _{β}	PA_{β}	c_3 (ECH): TPS $_{\beta}$	PA_{β}	c_3 (TPS-PMS): TPS $_{\beta}$	PA_{β}
[2/1]	21.7	21.7	35.1	35.1	35.1	35.1
[3/1]	13.7	15.7	19.5	22.9	19.0	21.5
[4/1]	11.1	15.8	14.4	20.8	13.1	18.7
[5/1]	9.3	16.9	11.2	19.6	8.8	17.3
[1/2]	12.8	12.8	17.3	17.3	17.3	17.3
[2/2]	12.4	14.9	16.9	20.4	16.2	19.4
[3/2]	$11.7 \pm 3.4 i$	15.8	$15.8 \pm 6.4 i$	$20.7 \pm 2.8i$	$15.4 \pm 7.4 i$	$17.3 \pm 3.6i$
[4/2]	$10.3 \pm 2.8i$	15.7	$12.9 \pm 5.1i$	$20.4 \pm 1.8i$	$11.6 \pm 6.8i$	$17.0 \pm 2.6i$
[1/3]	12.4	15.0	16.9	20.6	16.2	19.5
[2/3]	12.9	$15.1 \pm 1.2i$	17.4	19.3	$18.3 \pm 0.8i$	18.5
[3/3]	$10.6 \pm 2.9i$	$14.0 \pm 1.7i$	$13.6 \pm 5.5i$	$20.2 \pm 2.0 i$	$12.6 \pm 7.0 i$	$16.9 \pm 2.7i$

TABLE I. Predictions for c_3 in our, ECH and TPS-PMS approximants, using PA's of the invariant Borel transform $\overline{B}(z)$ of the approximants and demanding that the IR₁ pole be at $z_{\text{pole}} = 1/\beta_0$ (= 4/9). "TPS_{\beta}" denotes that the parameters $c_k^{(j)}$ ($k \ge 4$, j = 1, 2) in $\sqrt{A_{S^2}}$, and c_k ($k \ge 4$) in ECH and TPS-PMS, are set equal to zero; "PA_{\beta}" denotes that the \beta-functions in the approximants are resummed as: $[2/3]_{\beta}$ (RSch1); $[2/4]_{\beta}$ (RSch2; $c_4^{(2)} = c_4^{(1)}$); $[3/2]_{\beta}$ (ECH RSch, and TPS-PMS RSch).

analogous c_3 -fixing for the polynomial approximants ECH and TPS-PMS¹ to the BjPSR, and c_3 predictions for them are also included in Table I (columns with "TPS $_\beta$ "). These entries in the Table suggest the values $c_3 \approx 12.5, 17, 16$ for $\sqrt{A_{S^2}}$, ECH, and TPS-PMS, respectively. The predictions of PA $_{\overline{B}}$'s of intermediate order ([3/1], [4/1], [2/2], [3/2], [1/3], [2/3]) appear to give the most stable results. Predictions of the higher order PA $_{\overline{B}}$'s gradually lose predictability (predicted c_3 's can even become complex) because of the afore–mentioned overdetermination. The lowest order PA $_{\overline{B}}$'s are unreliable due to their too simple structure.

The possibility to adjust the N³LO coefficient r_3 of (14) in a similar way, was apparently first mentioned by the authors of Ref. [20]. They referred to PA's ([2/1]) of the simple Borel transform, so their (PA–resummed) predictions would depend on the choice of the RScl and RSch. A systematic method to optimize the perturbative expansion by including the information on the location of the IR₁ pole was suggested in Ref. [21].

¹ The ECH approximant is $\mathcal{A}_S^{(\text{ECH})}(c_3) = a(\ln Q_{\text{ECH}}^2; \rho_2, c_3, \ldots);$ the TPS-PMS approximant is $\mathcal{A}_S^{(\text{PMS})}(c_3) = a_{\text{PMS}} - \rho_2 a_{\text{PMS}}^3 / 2$, with $a_{\text{PMS}}(c_3) = a(\ln Q_{\text{ECH}}^2; 3\rho_2 / 2, c_3, \ldots), \ Q_{\text{ECH}}^2 = Q_0^2 \exp(-r_1/\beta_0).$

Up until now we have taken the higher order parameters $c_k^{(j)}$ $(k \ge 4, j = 1, 2)$ in our approximant (and in the ECH and TPS-PMS) to be zero, thus truncating the corresponding β -functions (TPS $_{\beta}$). However, since the considered observable has low process energy $Q_{\rm ph} \approx 1.73~{\rm GeV}$, we expect the higher order terms $\propto c_k^{(j)} x^{k+2}$ $(k \ge 4, x \equiv \alpha_s/\pi)$ of the β -function to contribute significantly to the determination (via evolution) of the relevant coupling parameters of the approximants. This leads us immediately to the question of quasianalytic continuation of the $\beta(x)$ functions from the small-x into the large-x regime. We can choose again Padé approximants (PA's) as a tool of this quasianalytic continuation, keeping c_3 as the only free parameter, and subsequently determine c_3 in the afore-mentioned way.

In $\sqrt{A_{S^2}}(c_3)$ there are β -functions characterized by the RSch-parameters $(c_2^{(1)}, c_3, \ldots)$ (RSch1) and $(c_2^{(2)}, c_3, ...)$ (RSch2) and determining the evolution and values of $a_1 \equiv$ $a(\ln Q_1^2; c_2^{(1)}, c_3, \ldots)$ and $a_2 \equiv a(\ln Q_2^2; c_2^{(2)}, c_3, \ldots)$, respectively. In the (NNLO) ECH and the TPS-PMS approximants, the RSch-sets are (ρ_2, c_3, \ldots) and $(3\rho_2/2, c_3, \ldots)$, respectively. For RSch1, ECH and TPS-PMS RSch, we have at first the freedom to construct [2/3], [3/2], or [4/1] PA_{β}'s. For RSch2, the additional condition $c_4^{(2)} = c_4^{(1)}$ ($\delta c_4 = 0$) has to be fulfilled. Since $c_4^{(1)}$ is a unique function of c_3 once a PA_{\beta1} choice has been made for RSch1, we then have for $PA_{\beta 2}$ of RSch2 the possibilities [2/4], [3/3], [4/2], [5/1]. For each choice of PA_{β} 's, we essentially repeat the afore-mentioned procedure of determining the value of c_3 . We consider the best choice of PA_{β} 's the one giving the most stable prediction of c_3 over various PA's $[M/N]_{\overline{B}}$ of the approximant's invariant Borel transform. This turns out to be for $\sqrt{A_{S^2}}(c_3)$ the choice $([2/3]_{\beta_1}, [2/4]_{\beta_2})$, although $([2/3]_{\beta_1}, [5/1]_{\beta_2})$ give virtually the same and almost as stable c_3 -predictions. For the ECH and TPS-PMS the choice is $[3/2]_{\beta}$. The predictions for c_3 are given in Table I (columns with "PA_{\beta}"). Those from PA's $[M/N]_{\overline{B}}$ of intermediate order are significantly more stable than the corresponding ones with truncated β -functions ("TPS_{\beta}"). This is a numerical indication that the PA-resummation of the \beta-functions improves the ability of the approximants to discern nonperturbative effects in the considered observable. The "PA_{\beta}"-entries in Table I give us approximate values $c_3 = 15.5, 20, 19$ for our, the ECH, and the TPS-PMS approximant, respectively.

There is yet another argument in favor of the above PA_{β} choices. The chosen $[2/3]_{\beta 1}$ and $[2/4]_{\beta 2}$ (or: $[5/1]_{\beta 2}$) have positive poles with mutually similar values: $x_{\text{pole}} = 0.334, 0.325$ (or: 0.291), respectively. The value of x_{pole} (= α_{pole}/π) indicates a point where "a strong and an asymptotically-free phase share a common infrared attractor" [22]. Thus, it is reasonable to expect that only those RSch's whose $\beta(x)$ -functions have about the same value of x_{pole} are suitable for the use in calculation of nonperturbative effects (on the other hand, in purely perturbative QCD, all RSch's are formally equivalent). Hence, the mutual proximity of x_{pole} 's of RSch1 and RSch2 PA_{\beta}'s is now yet another indication that these PA_{\beta}'s are the reasonable ones. What happens if we choose for RSch1 and RSch2 other PA_{β} 's? In such cases, we always end up with one of the following situations: Either the two corresponding positive x_{pole} values are far apart, or both values are unphysically small, or one (positive) x_{pole} doesn't exist, or there are no predictions for c_3 (not even unstable), or x_{pole} values are unstable under the change of c_3 in the interesting region $c_3 \approx 12$ –16. So, the choice $[2/3]_{\beta 1}$ and $[2/4]_{\beta 2}$ (or $[5/1]_{\beta 2}$) in our approximant is not just the choice giving the most stable c_3 -predictions, it is also the only choice giving mutually similar (and reasonable) values of x_{pole} of RSch1 and RSch2. Further, the choice $[3/2]_{\beta}$ for the ECH and TPS-PMS RSch's gives us x_{pole} values similar to the ones previously mentioned: $x_{\text{pole}} = 0.263$ for ECH with $c_3 = 20$; $x_{\text{pole}} = 0.327$ for TPS-PMS with $c_3 = 19$. Even other choices of PA_{β} for the ECH and TPS-PMS RSch's ($[2/3]_{\beta}$, $[4/1]_{\beta}$), which also give rather stable and very similar c_3 -predictions, give us $x_{\text{pole}} \approx 0.27$ -0.41. Therefore, we see in all cases a clear correlation between the stability of the c_3 -predictions on the one hand and $x_{\text{pole}} \approx 0.3$ -0.4 on the other hand. Finally, $[2/3]_{\beta}$ is then the good choice for $\overline{\text{MS}}$ RSch since it has $x_{\text{pole}} = 0.311$ ($c_3^{\overline{\text{MS}}}$, cf. Eq. (15), has been determined in Ref. [23]). The choices $[3/2]_{\beta}$ and $[4/1]_{\beta}$ for $\overline{\text{MS}}$ give $x_{\text{pole}} = 0.119$, 0.213, respectively, which are further away from 0.3-0.4.

Now that all the hitherto unknown parameters in $\sqrt{\mathcal{A}}$ of (4) and in the ECH and TPS–PMS have been determined, we use the approximants to predict the values of $\alpha_s^{\overline{\text{MS}}}(3\text{GeV}^2)$ (= πa_0) from the measured values of the BjPSR $S(Q_{\text{ph}}^2 = 3\text{GeV}^2)$. Experimental values at $Q_{\text{ph}} = \sqrt{3}$ GeV are given in [24] (their Table 4) and are based on SLAC data

$$\frac{1}{6}|g_A|\left[1 - S(Q_{\rm ph}^2)\right] = 0.177 \pm 0.018 \qquad \Rightarrow S(Q_{\rm ph}^2) = 0.155 \pm 0.086 \ . \tag{19}$$

where the constant $|g_A|$ is known [24] from β -decay measurements: $|g_A| = 1.257 \ (\pm 0.2\%)$. The experimental uncertainties are high, mainly because of the effects of perturbative evolution on the small- $x_{\rm Bi}$ extrapolation of the polarized structure functions appearing in the sum rule (13), as explained in Ref. [24]. We vary a_0 in our, and any other, approximant for the BjPSR S in such a way that the values (19) are reproduced. We then obtain the predictions for $\alpha_s^{\overline{\rm MS}}(3{\rm GeV}^2)$ given in Table II. Given are always three values for α_s , corresponding to the three values of S (19). The results are given for our, the ECH and the TPS-PMS approximants, all with the described c_3 -fixing and with the afore-mentioned PA-type resummation of the pertaining β -functions: $[2/3]_{\beta}$ (RSch1), $[2/4]_{\beta}$ (RSch2), $[3/2]_{\beta}$ (ECH), $[3/2]_{\beta}$ (TPS-PMS), $[2/3]_{\beta}$ (MS). Given are also predictions of such approximants when the β -functions are TPS's $(c_k^{(j)} = 0 \text{ for } k \geq 4)$. To highlight the importance of c_3 -fixing, we included predictions of these approximants (with TPS_{β}) when we set $c_3 = 0$ in them. In addition, predictions of the following approximants are included in Table II: TPS $S_{[2]}$ (14) (NNLO TPS); TPS $S_{[3]}$ with $r_3 = 128.05$ (N³LO TPS); off-diagonal Padé approximants $(PA's) [1/2]_S$ and $[2/1]_S$; square root of the diagonal PA $(dPA) [2/2]_{S^2}$, which is based solely on the TPS $S_{[2]}$ (14), as are the previous two off-diagonal PA's; $[2/2]_S$ is the dPA constructed on the basis of the N³LO TPS $S_{[3]}$ with $r_3 = 128.05$. For $[2/2]_S$ and N³LO TPS we took the value $r_3 = 128.05$ (in $\overline{\text{MS}}$, at RScl $Q_0^2 = 3\text{GeV}^2$) because then the [1/2] PA of the invariant Borel transform B_S (18) predicts the correct IR₁ pole $z_{\text{pole}} = 1/\beta_0$. Numbers in Table II are with four digits so that predictions of various methods can be easily compared.

Table II includes predictions for $\alpha_s^{\overline{\rm MS}}(M_Z^2)$. They were obtained from $\alpha_s^{\overline{\rm MS}}(3{\rm GeV}^2)$ by evolution via four–loop RGE, using the values of the four–loop $\overline{\rm MS}$ coefficient $c_3(n_f)$ [23] and the corresponding three–loop matching conditions [25] for the flavor thresholds. In the matching, we used the scale $\mu(n_f) = \kappa m_q(n_f)$ above which n_f flavors are active, with $\kappa = 2$, and $m_q(n_f)$ being the running quark mass $m_q(m_q)$ of the n_f 'th flavor. If increasing κ from 1.5 to 3, the predictions for $\alpha_s^{\overline{\rm MS}}(M_Z^2)$ decrease by at most 0.15%. If we use $[2/3]_\beta$ instead of TPS $_\beta$ in the evolution from 3GeV 2 to M_Z^2 , $\alpha_s^{\overline{\rm MS}}(M_Z^2)$ decreases by less than 0.04%.

In Fig. 1 we present various approximants as functions of $\alpha_s^{\overline{\text{MS}}}(M_Z^2)$. Our, ECH and TPS-PMS approximants have TPS β -functions and $c_3 = 12.5, 17, 16$, respectively (by the described IR₁ pole requirement). These three approximants, when the β -functions are

approximant	$\alpha_s(3~{\rm GeV}^2)$	$\alpha_s(M_Z^2)$
$\sqrt{A_{S^2}} \ (c_3 = 15.5; \ PA_{\beta}'s)$	$0.2755^{+0.0342}_{-0.1068}$	$\begin{array}{c} 0.1120^{+0.0047}_{-0.0219} \\ 0.1122^{+0.0051}_{-0.0221} \\ 0.1123^{+?}_{-0.0222} \end{array}$
ECH $(c_3 = 20.; PA_{\beta}'s)$	$0.2770^{+0.0371}_{-0.1082}$	$0.1122^{+0.0051}_{-0.0221}$
TPS-PMS $(c_3 = 19.; PA_{\beta}'s)$	$0.2778^{+?}_{-0.1090}$	$0.1123^{+?}_{-0.0222}$
$\sqrt{\mathcal{A}_{S^2}}$ ($c_3 = 12.5$; TPS _{β} 's)	$0.2798^{+0.0487}_{-0.1109}$	$\begin{array}{c} 0.1126^{+0.0064}_{-0.0224} \\ 0.1127^{+0.0066}_{-0.0225} \end{array}$
ECH $(c_3 = 17.; \text{TPS}_{\beta}\text{'s})$	$0.2801^{+0.0504}_{-0.1112}$	$0.1127^{+0.0066}_{-0.0225}$
TPS-PMS $(c_3 = 16.; \text{TPS}_{\beta}\text{'s})$	$0.2808^{+?}_{-0.1119}$	$0.1128^{+?}_{-0.0226}$
$\sqrt{\mathcal{A}_{S^2}} \ (c_3 = 0.; \text{TPS}_{\beta}\text{'s})$	$0.2853^{+0.0581}_{-0.1159}$	$0.1134^{+0.0073}_{-0.0231}$
ECH $(c_3 = 0.; \text{TPS}_{\beta}\text{'s})$	$0.2841^{+0.0573}_{-0.1148}$	$0.1133^{+0.0072}_{-0.0230}$
TPS-PMS $(c_3 = 0.; \text{TPS}_{\beta}\text{'s})$	$0.2848^{+7}_{-0.1155}$	$0.1133_{-0.0230}^{+0.0072} \\ 0.1134_{-0.0231}^{+?}$
$[2/2]_S \text{ (N}^3 \text{LO}, r_3 = 128.05)$	$0.2838^{+0.0595}_{-0.1147}$	$0.1132^{+0.0075}_{-0.0230}$
$\sqrt{[2/2]_{S^2}}$	$0.2832^{+0.0569}_{-0.1141}$	$0.1131^{+0.0071}_{-0.0229}$
$[2/1]_S$	$0.2890^{+0.0671}_{-0.1194}$	$0.1140^{+0.0080}_{-0.0237}$ $0.1145^{+0.0085}_{-0.0240}$
$[1/2]_S$	$0.2930^{+0.0727}_{-0.1230}$	$0.1145^{+0.0085}_{-0.0240}$
$N^3LO TPS (r_3 = 128.05)$	$0.2983^{+0.0855}_{-0.1281}$	$0.1152^{+0.0095}_{-0.0247}$
NNLO TPS	$0.3127^{+0.1021}_{-0.1403}$	$0.1171^{+0.0102}_{-0.0260}$

TABLE II. Predictions for $\alpha_s^{\overline{\rm MS}}$, derived from various resummations of the BjPSR at $Q_{\rm ph}^2 = 3 {\rm GeV}^2$. Predictions corresponding to $S_{\rm max} = 0.241$ cannot be made with the TPS-PMS, because the latter cannot be larger than $(2/3)^{3/2} \rho_2^{-1/2} \approx 0.233$, due to its specific polynomial form.

resummed by PA's, and $c_3 = 15.5, 20, 19$, respectively (IR₁ pole), are presented in Fig. 2. The three approximants with TPS_{β}'s (from Fig. 1) are included in Fig. 2 for comparison.

If we reexpand the approximants in powers of a_0 (RScl $Q_0^2 = Q_{\rm ph}^2$, in $\overline{\rm MS}$, $n_f = 3$), predictions for coefficient r_3 at a_0^4 of expansion (14) are obtained. Our approximant $\sqrt{\mathcal{A}_{S^2}}(c_3)$, with $c_3 = 15.5$, predicts $r_3 = 125.8 - c_3^{\overline{\rm MS}}/2 + c_3 \approx 130.8$, and the ECH $\mathcal{A}_S^{\rm (ECH)} = a(\ln Q_{\rm ECH}^2; \rho_2, c_3, \ldots)$, with $c_3 = 20$., predicts $r_3 = 129.9 + (-c_3^{\overline{\rm MS}} + c_3)/2 \approx 129.4$. Both predictions agree well with that of [26] $r_3 \approx 129.9$ (≈ 130 .) which was obtained from the ECH under the assumption $(-c_3^{\overline{\rm MS}} + c_3) \approx 0$ (note that $c_3^{\overline{\rm MS}} \approx 21.0$ was not known at the time [26] was written).

IV. DISCUSSION AND CONCLUSIONS

The results presented in Table II and in Figs. 1–2 show clearly that nonperturbative effects, as reflected in the mechanism of quasianalytic continuation from the small–a into large–a regime and in the presence of the leading infrared renormalon (IR₁) pole, play an important role in the BjPSR at low photon transfer momenta $Q_{\rm ph}\approx 1.73$ GeV. These effects decrease the predicted value of $\alpha_s^{\overline{\rm MS}}(M_Z^2)$ by very substantial amounts. Our approximant gives the BjPSR–prediction $\alpha_s^{\overline{\rm MS}}(M_Z^2)=0.1120^{+0.0047}_{-0.0219}$ (see Table II). Availability of additional data on polarized structure functions, especially in the low– $x_{\rm Bj}$ regime, may significantly reduce the uncertainties of the BjPSR–predictions for $\alpha_s^{\overline{\rm MS}}(M_Z^2)$.

The present world average is $\alpha_s^{\overline{\rm MS}}(M_Z^2) = 0.1173 \pm 0.0020$ by Ref. [27], and 0.1184 ± 0.0031

by Ref. [28]. The NNLO TPS predictions of the considered BjPSR (0.1171 $^{+0.0102}_{-0.0260}$, see Table II) cover the entire world average interval and more. However, when the afore–mentioned two classes of nonperturbative effects are taken into account, e.g. via the use of our or the ECH approximants and by the described c_3 –fixing, we obtain an upper bound $\alpha_s^{\overline{\text{MS}}}(M_Z^2)_{\text{max}} \approx 0.117$ – see Table II. But this upper bound does not surpass the central values of the afore–mentioned world averages. The central value of $\alpha_s^{\overline{\text{MS}}}(M_Z^2)$ extracted from the BjPSR (≈ 0.112) is significantly lower than the world average.

What could be the reason for this? One speculative possibility would be that some of the Feynman diagrams contributing to the N³LO term (yet unknown) of the BjPSR have a genuinely new topology not appearing in the lower diagrams, and that such new topology diagrams push the predicted values of $\alpha_s^{\overline{\text{MS}}}(M_Z^2)$ significantly upwards. The resummation methods based on the NNLO TPS cannot "foresee" such contributions [1,26]. In this context, we note that the afore–described c_3 –fixing in our, ECH and TPS–PMS approximants enables these approximants to be based on more than just the information contained in the NNLO TPS and in the RGE. However, since the location of the IR₁ pole can be determined by large– β_0 considerations, the described c_3 –fixing apparently does not incorporate information from those possible higher–loop diagrams whose topologies are genuinely new.

Another possible reason for the difference between our $\alpha_s^{\overline{\text{MS}}}$ -predictions and those of the world average could for example lie in a hitherto underestimated relevance of nonperturbative contributions and of higher order perturbative terms in the numerical analyses of data for some QCD observables. This possibility should be seen also in view of the fact that (some) NNLO contributions ($\sim a^3$) are not yet theoretically known for several of the quantities whose data have been analyzed to predict the world average [27,28]. However, lower values are allowed by some recent analyses beyond the NLO: $\alpha_s^{\overline{\text{MS}}}(M_Z^2) = 0.118 \pm 0.006$ [29] from the CCFR data for $x_{\text{Bj}}F_3$ structure function from νN DIS (NNLO); $0.112^{+0.009}_{-0.012}$ from Gross–Llewellyn–Smith sum rule [28] (NNLO); 0.115 ± 0.004 [27] from lattice computations.

From the theoretical point of view, we are dealing with three types of resummation approximants for NNLO TPS's of QCD observables in the present paper:

- 1. Padé approximants (PA's) provide an efficient mechanism of quasianalytic continuation. However, they do not possess RScl– and RSch–invariance, although their dependence on the RScl and on the leading RSch–parameter c_2 is in general weaker than that of the original TPS. In addition, they implicitly possess a c_3 –dependence, but this dependence has no special role since there is also c_2 and RScl–dependence.
- 2. Grunberg's ECH and Stevenson's TPS-PMS methods do not possess a strong mechanism of quasianalytic continuation, except the one provided by the RGE-evolution of the coupling parameter a itself.² This is so because these approximants do not go beyond the polynomial form in terms of the coupling parameter a. On the other hand, these approximants do achieve RScl- and c_2 -independence, since they represent a judicious choice of the RScl and of c_2 in the TPS. They possess a c_3 -dependence.

 $^{^2}$ In the one–loop limit, this amounts to the [1/1] PA quasianalytic continuation for a (ECH).

- 3. Our approximants provide an efficient mechanism of quasianalytic continuation, since they reduce to the diagonal PA expression $[2/2]_{S^2}^{1/2}$ in the one-loop limit (when all $c_k^{(0)}, c_k^{(j)}, c_k \mapsto 0$ for $k \geq 1$). At the same time, they possess invariance under the change of the RScl and of the leading RSch-parameter c_2 . They possess a c_3 -dependence.
- 4. The dependence on c_3 (and on c_k , $k \geq 4$) parameters in our, ECH and TPS-PMS approximants allows us to incorporate into them important nonperturbative information about the location of the leading IR renormalon pole. Further, it allows us to use in these approximants resummed β -functions (PA-type), thus presumably additionally strengthening the effects of quasianalytic continuation mechanism. These approximants are then fully independent of the RScl and RSch of the original TPS.

The leading higher–twist term contribution to the BjPSR ($\sim 1/Q_{\rm ph}^2$) [30]–[31], or a part of it, is implicitly contained in our approximant, as well as in the ECH and the TPS–PMS, via the afore–mentioned c_3 –fixing. The described approach implicitly gives an approximant–specific prescription for the elimination of the (leading IR) renormalon ambiguity. It is not clear which approximant accounts for the $\sim 1/Q_{\rm ph}^2$ terms in the best way.

A more detailed and extensive presentation of the subject will appear shortly [32].

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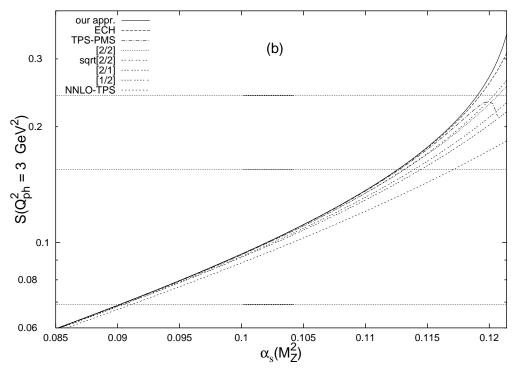


FIG. 1. Values of various approximants (of Table II) as functions of $\alpha_s^{\overline{\rm MS}}(M_Z^2)$. The β -functions in our, ECH and TPS-PMS approximants have TPS form and the values of c_3 in them were determined by the described IR₁ pole requirement. The experimental bounds (19) $S_{\rm min} = 0.069$, $S_{\rm max} = 0.241$ and $S_{\rm mid} = 0.155$ are indicated as horizontal lines.

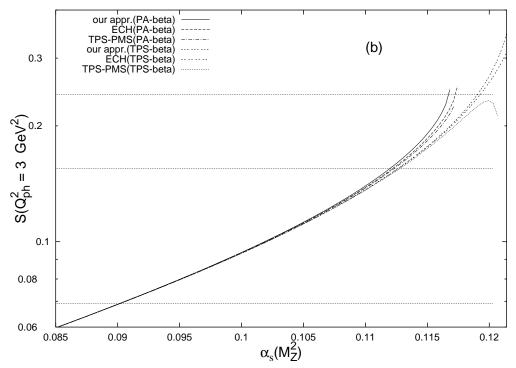


FIG. 2. As in Fig. 1, but the β -functions in our, ECH and TPS-PMS approximants are now resummed by PA's and the values of c_3 subsequently determined by the IR₁ pole requirement (see the text). For comparison, the corresponding predictions from Fig. 1, with TPS $_{\beta}$'s, are included.